

Single-crystal X-ray diffraction study on Al, H-bearing MgSiO₃T. Kuribayashi^{1,*}, T. Inoue², K. Fujino² and T. Nagase³¹Department of Earth Science, Graduate School of Science, Tohoku University, Sendai 980-8578²GRC, Ehime University, Matsuyama 790-8577³The Tohoku University Museum, Tohoku University, Sendai 980-8578**1. Introduction**

The perovskite-structured MgSiO₃ phase (Mg-Pv) is considered as a main component mineral of the earth's lower mantle, and is a key to understand the structural and physical properties of the earth's interior. This phase have been confirmed in a Tenham meteorite in 1997^[1], but in June 2014, at last, the phase was approved by the IMA-CNMNC, and was named bridgmanite, (Mg, Fe)SiO₃.

Crystal structure of Mg-Pv belongs to the orthorhombic system with space group of *Pbnm* (#62), and deviates from the ideal cubic perovskite structure. The Mg-Pv structure can include various minor components such as Ca, Fe, Al, and H etc. However, the information of the solubility of Al and H is poor. Recently, Mg-Pv including the larger amount of Al and H was synthesized at the conditions of 25-26 GPa and ~1600°C, and its incorporation mechanism (Si⁴⁺ ↔ Al³⁺ + H⁺) is suggested^[2]. However, structural information on (Al, H)-bearing Mg-Pv is unknown, and is needed to confirm the behaviors of Al and H in Mg-Pv structure.

So we conducted single-crystal X-ray diffraction measurements on (Al, H)-bearing Mg-Pv to obtain its structural information. In this report, we showed the brief results of X-ray diffraction experiments, and compared the lattice parameters of our sample with the previously reported values of the perovskite structure with various chemical formula.

2. Experimental Procedure

The sample used for this study was synthesized by Inoue et al. [2] at 25-26 GPa and ~1600°C. The run product included (Al, H)-bearing MgSiO₃ phase, phase D, stishovite and quenched dendritic phase, which was liquid under high pressure and temperature conditions. The chemical formula, Mg_{0.976}Si_{0.925}Al_{0.094}H_{0.089}O_{3*} of (Al, H)-bearing Mg-Pv was verified by [2] with EDS-SEM and SIMS. After checking the quality of crystals by taking oscillation photographs, a single crystal of Al, H-bearing Mg-Pv (56 μm × 48 μm × 40 μm in size) was selected for synchrotron X-ray diffraction experiments. Single crystal X-ray diffraction experiments were performed using the automated four-circle X-ray diffractometer installed at the beam line BL-10A, Photon Factory, High Energy Accelerator Research Organization. The wavelength (λ = 0.7129 Å) of synchrotron radiation was calibrated by the unit cell volume of the NIST ruby standard crystal at ambient temperature. The unit cell parameters of Al, H-bearing MgPv at room temperature were determined from

52 centered reflections in the 2θ range between 11° and 35°. The X-ray diffraction intensity data were collected up to sinθ/λ < 0.71 (2θ_{max} = 60°) by using ω-scan method.

3. Results and Discussion

The obtained lattice parameters of (Al, H)-bearing Mg-Pv are as follows: *a* = 4.7890(18) Å, *b* = 4.954(2) Å and *c* = 6.924(6) Å. Table 1 shows some lattice parameters of Mg-Pv with various minor components. Each axial length of (Al, H)-bearing Mg-Pv is expanded 0.3%, 0.5% and 0.4% compared with those of pure Mg-Pv[3]. The values of tilt angles defined by Zhao et al.[4] were almost same as those of pure Mg-Pv. The unit cell of (Al, H)-bearing Mg-Pv was isotropically expanded by the incorporation of Al and H. On the other hand, each axial length of (Fe, Al)-bearing Mg-Pv[5] is very closed to those of (Al, H)-bearing Mg-Pv. The axial lengths of Mg-Pv structure are strongly affected by the size of octahedron and the octahedral connection. These observations implied that the octahedral site is a key to understand the change of cell size and its incorporation mechanism. Now, the crystal structure of (Al, H)-bearing Mg-Pv is still in analysis.

Table 1. Unit cell parameters of our (Al, H)-bearing Mg-Pv and the reference data

Composition	This study (sample #1) Mg _{0.976} Si _{0.925} Al _{0.094} H _{0.089} O _{3*}	Horiuchi et al. (1987) MgSiO ₃	Dobson & Jacobsen (2004) MgSiO ₃	Vanpeteghem et al. (2006) Mg _{0.98} Si _{0.92} Al _{0.11} Fe _{0.02} O ₃
Unit Cell Parameters				
<i>a</i>	4.7890 (18)	4.7754 (3)*	4.7780 (2)	4.7820 (1)
<i>b</i>	4.954 (2)	4.9292 (4)*	4.9298 (3)	4.9422 (2)
<i>c</i>	6.924 (6)	6.8969 (5)*	6.8990 (3)	6.9207 (3)
<i>V</i>	164.25 (7)	162.35 (2)*	162.50 (1)	163.561 (1)
Tilt angles				
<i>cos φ</i>	12.0	11.7	11.6	12.3
<i>cos θ</i>	14.8	14.4	14.3	14.6
<i>cos φ</i>	19.0	18.4	18.3	19.0

*derived from Ito & Matsui (1978)

4. References

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